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Hamiltonian Formalism and the State of a Physical System

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Abstract—The purpose of this paper is to trace in a brief and readable manner, the evolution of mechanics from Newton to quantum mechanics. The key to the transition is the Hamiltonian formalism. We produce Hamilton's equations in special cases to give some sense of the importance and intrinsic interest in this formalism. Several examples are given to illustrate the power of the techniques. The idea of the "state" of a physical system is discussed and connections to quantum mechanics are made.

Keywords—Hamiltonian, Physical state, Lagrangian, Schrödinger equation.

1. INTRODUCTION

From Newton to the end of the 19th century, the agenda of reducing all physical phenomena to mechanics had gone from success to success. Add in the successes of Maxwell in electricity and magnetism and it may have seemed to some that physics was pretty much a finished subject. However, the beginning of the 20th century made it clear that there were problems when dealing with the composition of matter. The mechanics of Newton (1642–1727), later elegantly reformulated by Lagrange (1736–1813) and Hamilton (1805–1865), did very nicely in modeling macroscopic and astronomic motions. However, it failed in accounting for atomic phenomena. It was in the Cavendish laboratory in Cambridge, England, where many experiments on subatomic particles were first made. The little particles discovered there turned out to be decidedly non-Newtonian. Although the failure of Newtonian physics became evident at the atomic level, there are macroscopic phenomena that challenged the Newtonian view as well (see [1]). These failures led to the development of a new mechanics, quantum mechanics. It turns out that the Hamiltonian formulation rather than the Lagrangian formulation is the formalism that most readily generalizes to quantum mechanics via the Schrödinger equation. It is this evolution that we sketch in this paper, as well as the evolving concept of the "state" of a physical system.

2. NEWTON'S LAW AND THE STATE OF A PHYSICAL SYSTEM

When undergraduates are introduced to Newtonian mechanics, we usually begin by talking about an idealized *particle*, or "point mass". First, the particle must be somewhere in space, so

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we ascribe to it a *position vector* in $\mathbb{R}^3$ at any time t

$$\textit{position: } \vec{x} = \vec{x}(t) = (x_1(t), x_2(t), x_3(t)), \qquad \text{in } \mathbb{R}^3.$$

Second, we wish to describe the motion of the particle in space, so we ascribe a *velocity vector* and an *acceleration vector* to the particle

$$\textit{velocity: } \vec{v} = \vec{v}(t) = \frac{d\vec{x}}{dt} = \dot{\vec{x}}(t),$$
$$\textit{acceleration: } \vec{a} = \vec{a}(t) = \frac{d^2\vec{x}}{dt^2} = \ddot{\vec{x}}(t).$$

The law that governs the motion of the particle and which forms the basis for all of classical mechanics is the celebrated Newton's Second Law (see [2,3])

$$\vec{F}(\vec{x}) = m\ddot{\vec{x}} = m\frac{d^2\vec{x}}{dt^2}.$$

Here, of course, m is a constant of proportionality called *mass* and $\vec{F}$ is the *net force* acting on the particle. We can view $\vec{F}$ as a function of position $\vec{x}$ or time t, whichever is more convenient. Describing the motion of the particle amounts to solving for $\vec{x}(t)$, and so the natural mathematical language for classical mechanics is vector calculus and differential equations.

Newton's Second Law is a very powerful descriptive tool, due to the fact that the explicit form of the net force $\vec{F}$ can be written down in many interesting situations. In these instances, calculus methods can often be used to deduce the trajectory of the particle.

2.0.1. EXAMPLE. A FREE PARTICLE. Suppose a particle is very far away from everything else in the universe. Then for all intents and purposes,

$$\vec{F}(\vec{x}(t)) = \vec{0}.$$

It follows easily by integration that

$$\vec{v}(t) = \vec{v_0}, \qquad \text{a constant vector, and}$$
$$\vec{x}(t) = \vec{v_0}t + \vec{x_0}.$$

It thus follows that the motion of the particle will be along a straight line in space. This is just a mathematical statement of Newton's First Law: a moving body will travel in a straight line at constant speed unless acted upon by some external force.

2.0.2. EXAMPLE. A PARTICLE UNDER CONSTANT VERTICAL ACCELERATION. Suppose our particle is experiencing constant acceleration, say $\vec{g} = (0, 0, -g)$. For example, our particle might be experiencing the force of gravity in the vicinity of the earth's surface. Additionally, assume that our particle has an initial position $\vec{x}(0) = (0, 0, h)$ and initial velocity $\vec{v}(0) = (v_0 \cos\theta, 0, v_0 \sin\theta)$, where the angle θ is measured relative to the horizontal. Newton's Law says

$$m\vec{a} = m\vec{g} = m(0, 0, -g).$$

Integrating and evaluating arbitrary constants from the initial conditions, we find

$$\vec{v}(t) = (v_0 \cos\theta, 0, -gt + v_0 \sin\theta),$$
$$\vec{x}(t) = \left((v_0 \cos\theta)\, t, 0, -\frac{1}{2}gt^2 + (v_0 \sin\theta)\, t + h\right).$$

This says the trajectory of our particle is confined to the (x_1, x_3) plane. Moreover, if we write $t = x_1/(v_0 \cos\theta)$, we can eliminate t and find

$$x_3 = -\frac{1}{2}\frac{x_1^2}{v_0^2 \cos^2\theta} + x_1 \tan\theta + h.$$

This says the trajectory is parabolic.

A very important philosophical point arises from this mathematical formalism. Namely, if $\vec{F}(\vec{x})$ is known and if the values of $\vec{x}$ and $\vec{v}$ are given at *any one* time t_0, then the value of $\vec{x}$ is uniquely determined for *all* time t. Of course, there are some mathematical assumptions needed about $\vec{F}(\vec{x})$, but the exact restrictions need not concern us at this time. The main point is that we have a deterministic model of motion simply because Newton's Second Law takes the form of a second-order ordinary differential equation. So, given $\vec{x}(t_0)$ and $\vec{v}(t_0)$, $\vec{x}(t)$ is uniquely determined by the "equations of motion". But if we know $\vec{x}(t)$ for all t, we can compute $\vec{v}(t)$ for all t by differentiation. Thus, given the equation of motion, the values of $\vec{x}(t)$ and $\vec{v}(t)$ are uniquely determined by the values of $\vec{x}(t_0)$ and $\vec{v}(t_0)$, i.e., by the initial conditions.

Over time, physicists found it convenient to describe the behavior of a particle in terms of its position and *momentum* rather than its position and velocity. This change is essentially trivial since momentum $\vec{p}(t)$ is just mass times velocity

$$\textit{momentum: } \vec{p}(t) = m\vec{v}(t).$$

Then Newton's Law takes the form

$$\frac{d\vec{p}}{dt} = \vec{F}\left(\vec{x}(t)\right).$$

Thus, by our discussion above, given the equation of motion, the values of position $\vec{x}(t)$ and momentum $\vec{p}(t)$ are uniquely determined by the values of $\vec{x}(t_0)$ and $\vec{p}(t_0)$. We can now introduce the notion of the "state" of a particle at time t as follows:

> the state of a particle at time t is specified by giving the ordered pair of vectors $(\vec{x}(t), \vec{p}(t))$.

Thus, the state at time t can be considered a point in $\mathbb{R}^6$.

Now we can say that, given the equation of motion and the state at any time t_0, the state of the particle at any other time t is uniquely determined. Actually, the concept of a "state" is more general. We feel we have specified the state of the particle at time t if we have written down all information available about it at time t. Of course, this is somewhat vague, but it allows us to contemplate problems in which the amount of information available is limited for one reason or another, say because of experimental inaccuracy. For example, instead of knowing the initial conditions exactly, one might only have statistical, that is, probabilistic information; there are two functions $f(\vec{x}, 0)$ and $g(\vec{p}, 0)$ which are the probability density functions (pdfs) for the position and momentum at time 0.

So, if R and S are subsets of $\mathbb{R}^3$, all we could say is that the probability that $\vec{x}(0)$ is in R is $\int_R f(\vec{x}, 0)\, d\vec{x}$ and the probability that $\vec{p}(0)$ is in S is $\int_S g(\vec{p}, 0)\, d\vec{p}$. In this case, we say that the state of the particle at time $t = 0$ is specified by the functions $f(\vec{x}, 0)$ and $g(\vec{p}, 0)$. Thus, the state at time t will be specified by giving two probability density functions $f(\vec{x}, t)$ and $g(\vec{p}, t)$. Even with this "fuzziness", that is, "uncertainty", we can still assert that given the equation of motion and the state at time t_0, one can find the state at any time t. Again, this becomes a mathematical fact only under suitable assumptions on $\vec{F}$, f, and g given at time t_0.

For example, consider a free particle known to be located at the origin at time $t = 0$ with pdf $g(\vec{p}, 0)$ for its momentum. Since the particle is free, its momentum will be unchanged as it executes

its motion. Therefore, the pdf for momentum does not change with time; i.e., $g(\vec{p},t) = g(\vec{p},0)$ for all t. Now at time $t \neq 0$, we will not know the exact position of the particle. This is because we only had partial knowledge of its momentum at time $t = 0$ in the form of the pdf $g(\vec{p},0)$. So, even though we know the position exactly at time $t = 0$, we do not know exactly how fast and in what direction it is traveling, resulting in only partial knowledge of the position at later times. Thus, for times $t \neq 0$, our knowledge of the position is given by a pdf $f(\vec{x},t)$; i.e., $f(\vec{x},t)$ is the probability the particle is at $\vec{x}$ at time t. Roughly speaking, since we know the particle was at the origin at time $t = 0$, $f(\vec{x},t)$ must be proportional to the probability that the particle had the correct momentum to get from the origin to $\vec{x}$ in time t; i.e., $f(\vec{x},t) \propto g((m\vec{x}/t),0)$. Since $\int f(\vec{x},t)\,d\vec{x} = 1$ and $\int g(\vec{p},0)\,d\vec{p} = 1$, we find

$$f(\vec{x},t) = \left|\frac{m}{t}\right|^3 g\left(\frac{m\vec{x}}{t},0\right).$$

The concept of the "state of a physical system" as something which is specified by writing down all available information about the system is very general and not always clear. However, this idea arises over and over again in physical theories and one hopes to be able to take information about a system at one particular time and the equation of motion (the "theory") and be able to predict the state of the system at a later time.

3. ENERGY AND THE HAMILTONIAN

As the Newtonian formalism was applied to more and more complicated problems, it became clear that a more elegant and sophisticated approach was needed. This led to the reformulation of mechanics by Lagrange and Hamilton. There were also philosophical problems with the concept of force (see [4,5]). The concept of energy became central. In many problems, the net force $\vec{F}(\vec{x})$ turns out to be the gradient of a real-valued function (i.e., a scalar field). So we have

$$\vec{F}(\vec{x}) = -\nabla V(\vec{x}).$$

The scalar field $V(\vec{x})$ is called the *potential energy* of the particle at position $\vec{x}$. The force $\vec{F}$ is called *conservative* when it arises in this way. There are many mathematically equivalent ways of saying the force $\vec{F}$ is conservative (see [6,7]). Conservative systems arise frequently in physics, and their importance cannot be overemphasized. In fact, all of the physical systems considered in this article are conservative.

With these comments in mind, we continue. Physicists have found it useful to expand the concept of the energy E of a particle. We define a function of two vector variables $\vec{p}$ and $\vec{x}$ by

$$H(\vec{p},\vec{x}) = \frac{p^2}{2m} + V(\vec{x}),$$

where

$$p^2 = \vec{p}\cdot\vec{p}.$$

This function of two vector variables is called the *Hamiltonian* of the system. So far, this definition appears to have little to do with the motion of the particle. At this point, the vectors $\vec{p}$ and $\vec{x}$ are arbitrary vectors in $\mathbb{R}^3$ not necessarily having anything to do with our physical system. So let us now define the energy of a particle of momentum $\vec{p}(t)$ and position $\vec{x}(t)$ by

$$\textit{energy: } E(t) = \frac{p^2(t)}{2m} + V(\vec{x}(t)),$$

where $p^2(t) = \vec{p}(t)\cdot\vec{p}(t)$. The energy of our particle thus consists of two parts:

$$\textit{kinetic energy: } E_{\text{kin}}(t) = \frac{p^2(t)}{2m} = \frac{1}{2}mv^2(t), \text{ and the}$$
$$\textit{potential energy: } E_{\text{pot}}(t) = V(\vec{x}(t)).$$

A very important physical fact now becomes a mathematical theorem: *energy is conserved.* That is to say, $E(t)$ is a constant function of time. More precisely, if we have a conservative force and $\vec{p}(t) = m\vec{v}(t)$, then Newton's Second Law implies that $E(t) = E(t_0)$ for all t. Indeed, this is the reason for calling such a force $\vec{F}$ conservative.

The proof of this fact is not difficult and we give it next. Using familiar rules from vector calculus, we compute

$$\begin{aligned}\frac{dE}{dt} &= \frac{d}{dt}\frac{p^2(t)}{2m} + \frac{d}{dt}V(\vec{x}(t)) \\ &= \frac{\vec{p}(t)}{m}\cdot\frac{d\vec{p}}{dt} + \nabla V(\vec{x}(t))\cdot\frac{d\vec{x}}{dt} \\ &= \vec{v}(t)\cdot\left(\frac{d\vec{p}}{dt} + \nabla V(\vec{x}(t))\right) \\ &= \vec{v}(t)\cdot\left(\frac{d\vec{p}}{dt} - \vec{F}(\vec{x}(t))\right) = 0.\end{aligned}$$

Since the derivative of $E(t)$ is zero, $E(t)$ is constant.

The energy E thus provides us with a characteristic of the particle that does not change as the particle executes its motion. The conservation of the energy E turns out to be a simplifying principle in many interesting and complex problems and much attention has been focused on it for this reason. The Hamiltonian $H(\vec{p},\vec{x})$ has also been the subject of intense study because from this function, one can recover the equations of motion of the particle. In order to see this, we need to rewrite the equations of motion in terms of components x_1, x_2, x_3 and p_1, p_2, p_3 of position and momentum. We can write Newton's Law by

$$\frac{dp_i}{dt} = \dot{p}_i = F_i = -\frac{\partial V}{\partial x_i}, \qquad i = 1,2,3.$$

Now we can regard these three equations taken together as the equations of motion. However, if we compute the partial derivative of H with respect to x_i, we get

$$\frac{\partial H}{\partial x_i} = \frac{\partial V}{\partial x_i} \qquad i = 1,2,3,$$

so we see

$$\dot{p}_i = -\frac{\partial H}{\partial x_i}, \qquad i = 1,2,3.$$

Likewise, we find

$$\dot{x}_i = \frac{\partial H}{\partial p_i}, \qquad i = 1,2,3.$$

Thus, we can now regard these six equations as the equations of motion. These first-order partial differential equations, called *Hamilton's equations*, can be generalized to situations far more complicated than the one in which we have derived them, and indeed, all of classical mechanics can be formulated entirely in terms of Hamiltonians and Hamilton's equations of motion (see [3]).

We can now rewrite our previous statement about the determination of the state of a particle at any time by its state at one particular time as follows:

> given the Hamiltonian H and the state at time t_0, the state at any other time t is uniquely determined.

In writing this, we understand, of course, that the state at time t is to be determined by making use of Hamilton's equations of motion.

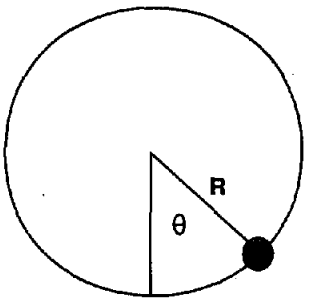

Figure 1.

3.0.3. EXAMPLE. THE SIMPLE PENDULUM. Consider a particle of mass m constrained to move along a circle of radius R while under the influence of gravity. The position of the particle is given by specifying the angle $\theta = \theta(t)$ of its location at time t (see Figure 1).

While Newton's Law is not completely transparent in this example, we easily produce the Hamiltonian by a good choice of coordinates, $H = H(p, \theta)$. First, $p = mR^2\dot{\theta}$ is the angular momentum and

$$H(p,\theta) = \frac{p^2}{2mR^2} + mgR(1 - \cos\theta).$$

The first of these terms is the kinetic energy due to the motion of the pendulum, while the second term is the potential energy of the system, due to the effect of gravity. Invoking Hamilton's equations, we see

$$\frac{d\theta}{dt} = \frac{\partial H}{\partial p} = \frac{p}{mR^2},$$

giving no new information, but

$$\frac{dp}{dt} = -\frac{\partial H}{\partial \theta}.$$

Therefore,

$$mR^2\frac{d^2\theta}{dt^2} = -mgR\sin\theta.$$

This gives us the differential equation which determines the motion of the particle

$$\frac{d^2\theta}{dt^2} + \left(\frac{g}{R}\right)\sin\theta = 0.$$

3.0.4. EXAMPLE. THE HARMONIC OSCILLATOR. Consider a particle of mass m attached to a spring (see Figure 2). The problem is to determine the motion of the mass if we stretch the spring horizontally and then let go.

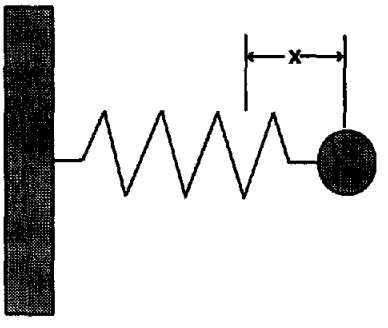

Figure 2.

To do so, let x be the displacement of the mass from its position in equilibrium. The stiffness of the spring is measured by a constant κ, and the spring is assumed to produce a linear restoring force. As a consequence, the potential energy function is given by $V(x) = (1/2)\kappa x^2$. The resulting Hamiltonian for the system is then $H(p, x) = p^2/2m + (1/2)\kappa x^2$. Hamilton's equations read

$$\dot{p} = -\frac{\partial H}{\partial x} = -\kappa x$$

and

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}.$$

Recalling that $\dot{p} = m\ddot{x}$, the first equation tells us that

$$\ddot{x} = -\frac{\kappa}{m}x,$$

which is just Newton's Second Law for our mass and spring system. Solving the differential equation yields

$$x(t) = A\sin(\omega t + B),$$

where

$$A, B \in \mathbb{R}, \qquad \omega = \sqrt{\frac{\kappa}{m}}.$$

Therefore, the system will undergo periodic motion and the constant ω, known as the *angular frequency* of the system, determines the rapidity of the oscillations.

Next let us consider a more challenging problem.

3.1. EXAMPLE. AN ELASTIC PENDULUM. Consider a particle of mass m attached to the end of an elastic pendulum of natural length L. Let $x = x(t)$ denote the (stretched) length of the arm at any time t (see Figure 3).

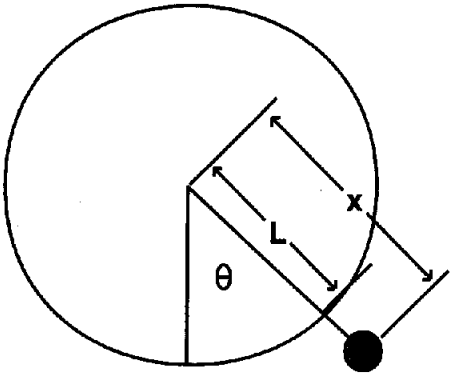

Figure 3.

Then the tension T is

$$T = -\frac{E(x - L)}{L},$$

where E is the modulus of elasticity of the material of the arm. Then if θ measures the angle between the arm and the vertical, we find that the potential energy is $-mgL\cos\theta + (1/2)(E(x - L)^2)/L$, while the kinetic energy is $(1/2)m(\dot{x}^2 + x^2\dot{\theta}^2)$, so the Hamiltonian is

$$H = \frac{1}{2}m\left(\dot{x}^2 + x^2\dot{\theta}^2\right) - mgL\cos\theta + \frac{1}{2}\frac{E(x - L)^2}{L}.$$

Hamilton's equations lead to two ordinary differential equations

$$mx^2\ddot{\theta} + 2mx\dot{x}\dot{\theta} + mgL\sin\theta = 0,$$

$$m\ddot{x} - mx\dot{\theta}^2 + \frac{E}{L}(x - L) = 0,$$

as the reader may verify.

4. CLASSICAL MECHANICS FOR n PARTICLES

The equations of motion for a system of n particles are a straightforward generalization of the equations for one particle. One introduces position vectors for each of the n particles, $\vec{x_1}(t), \vec{x_2}(t), \ldots, \vec{x_n}(t)$, and writes

$$m_l \ddot{\vec{x}}_l(t) = \vec{F}_l\left(\vec{x_1}(t), \vec{x_2}(t), \ldots, \vec{x_n}(t)\right), \qquad l = 1, 2, \ldots, n.$$

Here we have called explicit attention to the fact that the force on particle l may depend not only on its own position, but on the positions of all the other particles as well. A case of particular interest is the case in which the force acting on particle l is produced by its interaction with all the other particles. Writing $\vec{F}_{l_j}$ for the force exerted on particle l by particle j, we have

$$m_l \ddot{\vec{x}}_l(t) = \sum_{j \neq l} \vec{F}_{l_j}(\vec{x_l}(t), \vec{x_j}(t)).$$

Newton's Third Law tells us that the force on particle l due to particle j should be equal in magnitude and opposite in direction to the force on particle j due to particle l; i.e., we have

$$\vec{F}_{j_l} = -\vec{F}_{l_j}.$$

Now this will be satisfied automatically if, as often turns out, the forces $\vec{F}_{j_l}$ are derivable from potentials $V_{jl} = V_{lj}$ which are functions of the difference between $\vec{x}_i$ and $\vec{x}_l$. We now assume this to be the case, that is, we assume only two-body interactions.

$$V_{jl} = V_{jl}\left(\vec{x}_j - \vec{x}_l\right)$$

and

$$\vec{F}_{l_j} = -\nabla_l V_{jl}\left(\vec{x}_j - \vec{x}_l\right),$$
$$\vec{F}_{j_l} = -\nabla_j V_{jl}\left(\vec{x}_j - \vec{x}_l\right).$$

Now define a potential V which is the sum over all pairs of distinct particles

$$V\left(\vec{x_1}, \vec{x_2}, \ldots, \vec{x_n}\right) = \sum_{j<l} V_{jl}\left(\vec{x}_j - \vec{x}_l\right).$$

Then one computes

$$-\nabla_l V\left(\vec{x_1}, \vec{x_2}, \ldots, \vec{x_n}\right) = \sum_{j \neq l} \vec{F}_{l_j} = \vec{F}_l.$$

Thus,

$$-\nabla_l V\left(\vec{x_1}(t), \vec{x_2}(t), \ldots, \vec{x_n}(t)\right) = m_l \ddot{\vec{x}}_l(t).$$

Defining the momentum of the l^{th} particle by

$$\vec{p}_l(t) = m_l \dot{\vec{x}}(t),$$

we have

$$\dot{\vec{p}}_l(t) = -\nabla_l V.$$

As before, we define a Hamiltonian by

$$H\left(\vec{p}_1, \vec{p}_2, \ldots, \vec{p}_n; \vec{x_1}, \vec{x_2}, \ldots, \vec{x_n}\right) = \sum_{l=1}^{n} \frac{p_l^2}{2m_l} + \sum_{j<l} V_{jl}\left(\vec{x}_j - \vec{x}_l\right).$$

As before, we can prove that energy is conserved. That is,

$$E(t) = H\left(\vec{p}_1(t), \vec{p}_2(t), \ldots, \vec{p}_n(t); \vec{x}_1(t), \vec{x_2}(t), \ldots, \vec{x_n}(t)\right)$$

is constant if $\vec{x}_l(t)$ and $\vec{p}_l(t)$ are related as above.

Finally, we can show that these relations are equivalent to the $6n$ equations

$$\dot{p}_l^\alpha = -\frac{\partial H}{\partial x_l^\alpha},$$
$$\dot{x}_l^\alpha = -\frac{\partial H}{\partial p_l^\alpha},$$

where $\alpha \in \{1, 2, 3\}$ designates one of the components of the corresponding three vectors, and $l \in \{1, 2, \ldots, n\}$ ranges over the total number of particles. The following example indicates the ease with which interesting physics can be predicted from these techniques.

4.0.1. EXAMPLE. COUPLED HARMONIC OSCILLATORS. This example is intended to illustrate Hamilton's equations for multiparticle systems. For a more thorough discussion, see the book by Fowles [8], from which the following presentation is adapted.

Consider a system of two balls of mass m attached to springs, both with spring constants κ. Additionally, we assume that they are attached to each other by a spring of strength κ' (see Figure 4). If the system is disturbed from equilibrium, how can we describe the resulting motion?

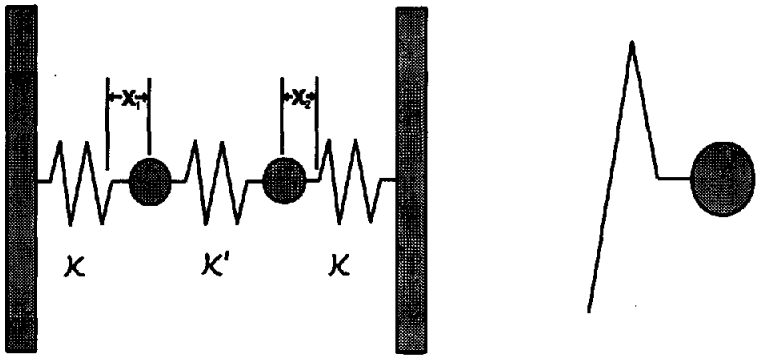

Figure 4.

To analyze this system, we let x_1 and x_2 represent the displacement of the balls from their respective equilibrium positions. The momentum of the two balls is given by p_1 and p_2, respectively. Recalling the expression for potential energy given in the previous example, we see that the Hamiltonian for this system is given by

$$H\left(p_1, p_2; x_1, x_2\right) = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}\kappa x_1^2 + \frac{1}{2}\kappa x_2^2 + \frac{1}{2}\kappa'\left(x_2 - x_1\right)^2,$$

since the distance that the middle spring has been stretched is $x_2 - x_1$. Hamilton's equations for the momentum variables then read

$$m\ddot{x}_1 = \dot{p}_1 = -\kappa x_1 + \kappa'\left(x_2 - x_1\right),$$
$$m\ddot{x}_2 = \dot{p}_2 = -\kappa x_2 - \kappa'\left(x_2 - x_1\right).$$

Using the single harmonic oscillator as a guide for what might happen in this case leads us to try a solution of the form

$$x_1(t) = A\sin(\omega t),$$
$$x_2(t) = B\sin(\omega t),$$

where ω is undetermined. This leads, by substitution, to

$$\begin{aligned}\left(-mA\omega^2 + \kappa A - \kappa'(B-A)\right)\sin(\omega t) &= 0,\\ \left(-mB\omega^2 + \kappa B + \kappa'(B-A)\right)\sin(\omega t) &= 0.\end{aligned}$$

This will be satisfied if the coefficients are both zero; that is, if

$$\begin{aligned}\left(-m\omega^2 + \kappa + \kappa'\right)A - \kappa' B &= 0,\\ -\kappa' A + \left(-m\omega^2 + \kappa + \kappa'\right)B &= 0.\end{aligned}$$

We can view this as a linear system of equations in the variables A and B. If we are to have any motion in our physical system, then the above system of equations must have a nontrivial solution. This requires

$$\det\begin{bmatrix} -m\omega^2 + \kappa + \kappa' & -\kappa' \\ -\kappa' & -m\omega^2 + \kappa + \kappa' \end{bmatrix} = 0.$$

Expanding the determinant and solving for ω yields the *two* solutions

$$\omega_s = \sqrt{\frac{\kappa}{m}} \qquad \text{and} \qquad \omega_a = \sqrt{\frac{\kappa + 2\kappa'}{m}}.$$

Thus, there are two special frequencies, known as *normal frequencies*, for this system. It should be noted that the above linear system for A and B yields $A = B$ if $\omega = \omega_s$ and $A = -B$ if $\omega = \omega_a$. For this reason, the solution with $\omega = \omega_s$ is known as the *symmetric mode*, while the solution with $\omega = \omega_a$ is known as the *antisymmetric mode*. As would be expected, the general solution for this system is given by

$$\begin{aligned}x_1(t) &= A\sin(\omega_s t + a) + B\sin(\omega_a t + b),\\ x_2(t) &= A\sin(\omega_s t + a) - B\sin(\omega_a t + b),\end{aligned}$$

where A, B, a, and b are real numbers determined by the initial conditions of the system. Solutions with contributions only from the symmetric mode or the antisymmetric mode are known as the *normal modes* of the system.

5. WHY THE HAMILTONIAN FORMALISM?

First, we note that there is another approach to classical mechanics known as the Lagrangian formulation. In this framework, one begins by finding the Lagrangian L, which is the *difference* between the kinetic and potential energies. One then calculates the "action integral"

$$\begin{aligned}J(\vec{x}) &= \int_{t_0}^{t_1} L(\vec{x}(s))\, ds\\ &= \int_{t_0}^{t_1} \left[\frac{1}{2}m\left|\frac{d\vec{x}}{dt}(s)\right|^2 - V(\vec{x}(s))\right] ds.\end{aligned}$$

Here the domain of J consists of (suitably smooth) paths joining fixed points $\vec{x}(t_0)$ and $\vec{x}(t_1)$. The trajectories that make this action integral stationary with respect to variations in the path are precisely those that obey Newton's Second Law, as can be shown by standard techniques in the calculus of variations. The equations of motion derived by this method are known as the *Euler-Lagrange equations*, and have a simple expression in terms of the Lagrangian (see Table 1). This method is just as successful for mechanics as the Hamiltonian formalism, and many classical texts adopt this approach (see [3,9]).

Considering that we have discussed three separate (and seemingly equally successful) approaches to classical mechanics, one has to wonder why focus on the Hamiltonian formalism. There are several answers to this question, some based on mathematical reasons and others based on physical ones. We mention three sources of our motivation. First, at a practical level, the Hamiltonian approach is easily adapted to "generalized coordinates", which allows the equations of motion to be more easily obtained. Second, from the mathematical point of view, the natural mathematical setting for classical mechanics is the study of *symplectic manifolds*, in which the dynamics is given by the Hamiltonian formalism. Finally, from both a physical and mathematical perspective, the abstract study of *quantization* involves the starting data of a symplectic manifold, or equivalently, a classical mechanical system described by the Hamiltonian formalism. This is perhaps the most compelling physical argument supporting the Hamiltonian approach as fundamental. In what follows, we sketch the historical connection between the Hamiltonian formalism and nonrelativistic quantum mechanics.

Around the turn of the century, physicists' experimental sophistication had grown to the point that they could begin to study the structure of the atom. To their surprise, many experiments produced results that could not be predicted from classical mechanics. In particular, classical mechanics did not even predict a stable atom! It became quite clear that Newtonian physics was fundamentally flawed in its description of the microscopic. In the years that followed, physicists developed the theory of quantum mechanics to explain their new observations.

Historically, it turned out that the transition from classical mechanics, which demonstrably fails at the subatomic level, to quantum mechanics was much easier to make within the framework of the Hamiltonian formalism. In quantum mechanics, there is still something called a Hamiltonian (an operator obtained by analogy from the classical Hamiltonian function) and given the Hamiltonian, it is still true that if one knows the state at time t_0, one can find the state at any other time t. This is the primary goal of elementary quantum mechanics texts (see, for example, [10,11]). However, there is a significant difference. One does not mean the same thing by a "state" in quantum mechanics that one means in classical mechanics. Likewise, one does not mean the same thing by a Hamiltonian. Furthermore, the equation of motion is not the same. Instead of using the familiar Second Law of Newton, one writes down the Schrödinger equation.

In 1927, Davisson and Germer used X-ray diffraction of electrons by crystals to decisively demonstrate the wave nature of matter. In quantum mechanics, this wave behavior is described by specifying a particle's "wave function", and it is this wave function that determines the state of a quantum mechanical system. In the early wave theory of matter proposed by de Broglie, a particle has a wavelength related to its momentum by the formula $\lambda = h/p$, where h is Planck's constant. Now suppose an electron of mass m is traveling with velocity v, and hence, momentum $p = mv$ in field free space. With no forces acting on the electron, we expect ψ, the wave function of the electron, to be a plane wave of the form

$$\psi(x,t) = Ae^{i(kx-\omega t)},$$

where $k = 2\pi$, λ, and $\omega = 2\pi\nu$, with λ being the wavelength and ω the frequency. Einstein proposed the relationship $E = h\nu$ in his theory of the photoelectric effect, where E is the energy of a particle. Using this formula and the de Broglie wavelength-momentum relationship allows one to write

$$k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} \qquad \text{and} \qquad \omega = 2\pi\nu = \frac{2\pi E}{h}.$$

Thus, we may rewrite the wave function as

$$\psi(x,t) = Ae^{i((2\pi px)/h-(2\pi Et)/h)}.$$

Simple differentiation yields

$$\frac{\partial\psi}{\partial t} = -\frac{2\pi iE}{h}\psi, \qquad \text{so } i\left(\frac{h}{2\pi}\right)\frac{\partial\psi}{\partial t} = E\psi.$$

Also,

$$\frac{\partial \psi}{\partial x} = \frac{2\pi i p}{h}\psi, \qquad \text{so} \quad \left(\frac{h}{2\pi i}\right)\frac{\partial \psi}{\partial x} = p\psi.$$

Differentiating again, we find that

$$\begin{aligned}\frac{\partial^2 \psi}{\partial x^2} &= -\left(\frac{2\pi p}{h}\right)^2 \psi \\ &= -\left(\frac{2\pi}{h}\right)^2 \left(\frac{p^2}{2m}\right)(2m)\psi \\ &= -\left(\frac{2\pi}{h}\right)^2 \left(\frac{1}{2}mv^2\right)(2m)\psi \\ &= -\left(\frac{2\pi}{h}\right)^2 (2mE)\psi, \qquad \text{so} \\ -\frac{1}{2m}\left(\frac{h}{2\pi}\right)^2 \frac{\partial^2 \psi}{\partial x^2} &= E\psi.\end{aligned}$$

Letting $\hbar = h/2\pi$, we obtain the following equation:

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}.$$

If the electron is under the influence of a potential V, this equation is modified to obtain the well-known Schrödinger equation

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi.$$

This motivates the famous equation that serves as the starting point for the theory of nonrelativistic quantum mechanics. In several dimensions, it reads

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi.$$

The Schrödinger equation can be an enigma to people trained in classical mechanics. One has an intuition for what Newton's Second Law means. If you push something, it starts moving! The Schrödinger equation, on the other hand, is not intuitive. What is a wave function and what does the Schrödinger equation mean? In quantum mechanics, the "intensity" of a wave function ψ is given by $|\psi|^2$, and this function is interpreted as a pdf for the position of the particle. The Schrödinger equation determines the time evolution of the wave function. Certainly the wave function, and its interpretation as a pdf, is not an intuitive concept! One would, of course, be willing to put up with this if the Schrödinger equation were just a rather complicated mathematical consequence of some familiar results of classical mechanics. One could then argue that if you believe some reasonable assumptions and deduce the Schrödinger equation, then you just have to accept it. However, the Schrödinger equation was *not* deduced from the laws of classical mechanics and there are reasons to believe that it *cannot* be so deduced (see [12]). However, interpreting the wave function as a pdf (from which the pdfs for momentum, energy, etc., can be determined), has led to a very successful description of atomic behavior. With such wonderful agreement between experiment and the quantum theory, one is forced to concede the macroscopic intuition in Newton's Law for the successful though less intuitive Schrödinger equation.

We regard the Schrödinger equation not as something which ought to be deducible from the "old" formalism, but as a new point of departure with implications different from those of Newton's Second Law. This was the role that the equation played historically. It is true that the

"meaning" of the equation is not immediately apparent. The implications help us to see the meaning. We emphasize again that Newton' Second Law actually predicts something false which can be remedied within the framework of quantum mechanics. So if the Schrödinger equation does not seem intuitively plausible, remember that the phenomena it was intended to predict and describe were not plausible from the classical point of view.

We close with the following table, summarizing the differences between the various approaches to classical and quantum mechanics. In what follows, $T = T(\vec{x}, \vec{p})$ is the kinetic energy, V is the potential energy, ψ is a wave-function (a complex-valued function defined on $\mathbb{R}^n$), and $\nabla^2 = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$ is the Laplacian.

Table 1.

Classical Mechanics		
Newtonian Approach	Lagrangian Approach	Hamiltonian Approach
Newton's Law $\vec{F} = m\vec{a}$	Lagrangian $L = T - V$ Euler Lagrange equations $\frac{d}{dt}\left(\frac{\partial L}{\partial p_i}\right) - \frac{\partial L}{\partial x_i} = 0$	Hamiltonian $H = T + V$ Hamilton's equations $\dot{p}_i = -\frac{\partial H}{\partial x_i}$ $\dot{x}_i = \frac{\partial H}{\partial p_i}$

Quantum Mechanics
Hamiltonian: $H = -\frac{\hbar^2}{2m}\nabla^2 + V$
Schrödinger equation: $i\hbar\frac{\partial \psi}{\partial t} = H\psi$

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